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Renormalization group in quantum mechanics at zero and finite temperature

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We apply the renormalization group formalism, to integrate quantum fluctuations of quantum mechanical systems at zero and finite temperature. At zero temperature a nonperturbative renormalization group equation allows to compute the ground state energy whereas at finite temperature a variational renormalization group equation is proposed to compute the free energy.

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I. INTRODUCTION

Methods of reducing quantum statistical calculations to classical ones are very important from theoretical and practical point of view. In this context the path integral approach has been proved to be very useful, as the quantum partition function can be approximated by a classical one after integration of the quantum fluctuations. Several methods based on a variational principle have been proposed to compute these quantum fluctuations [1,2] leading to an effective classical potential. In particular the Feynman-Kleinert [3,4] variational approach has shown to give accurate results and to be easy to handle. Later this method has been improved by the variational perturbation theory [4,5,6], but computations get rapidly cumbersome with the perturbation expansion.

In previous papers [7,8,9] we proposed an alternative method based on the renormalization group (RG) to integrate the quantum fluctuations and to obtain the effective classical potential. This procedure is nonperturbative and nonvariational. It has proven to be very efficient and easy to handle for the computation of the ground state and first excited energy level of a one quantum particle system at zero temperature. Moreover it allows to find with a greater accuracy than the variational method the particle distribution [9]. Unfortunately this method seemed not to be really promising for finite temperature calculus.

The aim of the present paper is twofold. In the first part we apply the zero temperature RG formalism to several different physical models. Even if the RG method cannot compete with the efficiency of Kleinert's systematic variational perturbation that converge to the exact result [4,5,6], it has the merit to be easily extrapolated to nonpolynomial potentials and to systems of particles in interaction. We then compute the ground state and the first excited energy level for a one quantum particle in the sextic potential and discuss the convexity of the effective classical potential of a particle in a periodic cosine potential. In addition we derive the RG equation for a two quantum particles in interaction system and apply it to a pair of coupled oscillators with quartic couplings. Our results are very accurate for small couplings and accurate to a few percent for large couplings.

In a second part we inspect more carefully the finite temperature case. It is well known that the zero temperature RG equation takes automatically into account, through the running coupling constants, all the terms in the loop expansions. In Ref. [7] it has been found that this is no more the case in finite temperature as the RG equation is no more a closed expression but is defined by an infinite series in the temperature. We have studied the flow of the coupling constants by truncating this RG series. But the results being not convincing we turn to an improvement of the variational Feynman-Kleinert method by the renormalization group, the goal being to automatically resum terms of the variational perturbation theory, as already suggested in Ref. [7]. We find only an improvement of the Kleinert variational perturbation expansion for small values of the coupling and large temperature, but our results cannot compete for strong coupling. We discuss the reasons for these mitigated results.

Section II is devoted to the zero temperature situation. In Sec. II A, to establish clearly the formalism, we apply the RG method to the sextic oscillator. The case of the one quantum particle in a periodic cosine potential is developed in Sec. II B. In Sec. II C, as a generalization of the previous formalism, we establish the RG equation for two particles with an arbitrary interaction and obtain quantitative results for a pair of coupled oscillators with quartic couplings.

In Sec. III we investigate the finite temperature situation. Section III A is devoted to the study of the truncation of the RG finite temperature series. The variational RG equation is derived in Sec. III B and applied to the computation of the free energy for the anharmonic oscillator.

II. RENORMALIZATION GROUP AT ZERO TEMPERATURE

In this section we recall the main steps of the procedure leading to the RG equation in quantum mechanics. We work in the euclidean formalism at a finite temperature and discrete time and quickly retrieve the RG equation as was done in Ref. [8]. In this section we limit ourself to the zero temperature limit, so we will always neglect contributions of order $1/\beta^2$. Keeping a finite temperature in the intermediary steps allows to work with a finite number of Fourier modes, so that we can integrate each mode after the other in the path integral.

Consider the euclidean action of a quantum particle at a finite temperature

$$S(x)=\int_0^{\hbar\beta}\left[\tfrac{1}{2}M\left(\frac{d}{dt}x(t)\right)^2+V(x(t))\right], \tag{1}$$

with M the mass and V the potential.

The effective classical potential is defined as a constrained path integral over periodic paths with period $\hbar\beta$ [4]

$$\exp[-\beta V_0(x_0)]=\int \mathcal{D}x\,\delta(\overline{x}-x_0)\exp\left[-\frac{1}{\hbar}S(x)\right], \tag{2}$$

where $\overline{x}=1/\hbar\beta\int_0^{\hbar\beta}dt\,x(t)$ is the average position of the particle in the time interval $t\in[0,\beta]$.

We consider the Feynman path integral with a discretized time $t_n=nT/N+1=n\epsilon$, with N an arbitrary large number, and $n=0,\ldots,N+1$. The Fourier decomposition of a periodic path $x(t_n)$ contains only a finite number of Fourier modes

$$x(t_n)=x_0+\frac{1}{\sqrt{N+1}}\sum{}' \exp(i\omega_m t_n)x_m+\text{H.c.}, \tag{3}$$

where Σ' is from 1 to $N/2$ if N is even and from 1 to $N-1/2$ if N is odd. The x_m are the Fourier modes and

$$\omega_m^2=\frac{2-\cos\dfrac{2\pi m}{N+1}}{\epsilon^2}.$$

The discrete action is [4]

$$S_{N/2}(x)=\epsilon\sum_0^{N/2} N\omega_m^2|x_m|^2+\epsilon\sum_{n=l}^{N+1} V_{N/2}(x(t_n)) \tag{4}$$

and the partition function,

$$Z=\int\frac{dx_0}{\sqrt{2\pi\hbar\epsilon/M}}\int\prod_1^{N/2}\frac{dx_m\,d\overline{x}_m}{\dfrac{2\pi\epsilon\hbar}{M}}\exp\left(-\frac{1}{\hbar}S_{N/2}\right). \tag{5}$$

Now, using the fact that $\Pi_1^{N/2}\epsilon^2\omega_m^2=\sqrt{N+1}$ (see [4]) and $\hbar\beta=(N+1)\epsilon$, we can drop the first integral to get the effective classical potential [4]:

$$\exp(-\beta V_0(x_0))=\int\prod_1^{N/2}\frac{dx_m\,d\overline{x}_m}{\dfrac{2\pi\epsilon\hbar}{\epsilon^2\omega_m^2 M}}\exp\left(-\frac{1}{\hbar}S_{N/2}\right). \tag{6}$$

The RG method allows to compute V_0 by integrating recursively, each mode after the other in the path integral. Let

$$x^{(m)}(t_n)=x_0+\frac{1}{\sqrt{N+1}}\sum_{p=1}^{m}\exp(i\omega_p t_n)x_p+\text{H.c.}, \tag{7}$$

the truncated path with Fourier components up to m (the so called background path). We define the running action at step $m-1$, S_{m-1}, recursively by integrating on the two modes x_m and $\overline{x_m}$ that is

$$\exp\left[-\frac{1}{\hbar}S_{m-1}(x^{(m-1)})\right]=\int\frac{dx_m\,d\overline{x_m}}{\dfrac{2\pi\epsilon\hbar}{\epsilon^2\omega_m^2 M}}\exp\left[-\frac{1}{\hbar}S_m(x^{(m)})\right], \tag{8}$$

where $S_{N/2}$ is the initial action.

Note an important point observed in Ref. [8]. Only a kind of quasilocal potential is preserved by the renormalization group flow (8). As shown in Ref. [8] we have to consider for the potential V_m a function of the $m+1$ independent variables $V_m(x_0,\ldots,x_p e^{i\omega_p t}+x_{-p}e^{i\omega_p t},\ldots,e^{i\omega_m t}x_m+e^{i\omega_m t}x_{-m})$ denoted for convenience by $V_m(x^{(m)}(t))$.

In fact, due to the nonlinearity of the ω_m, this kind of potential is not preserved by the RG flow. But recall that we want to consider the limit $\beta\rightarrow\infty$. In such limit $\omega_m=2\pi m/\hbar\beta$ and the class of function considered is preserved by the flow.

To derive the flow equation for the potential, it is easier to work in functional space. We write the action at scale m

$$S_m(x^{(m)})=\epsilon\sum_{p=0}^{m} M\omega_p^2|x_p|^2+\beta U_m(x^{(m)}), \tag{9}$$

where we have introduced the notation

$$U_m(x^{(m)})=\frac{\epsilon}{\beta}\sum_{n=0}^{N+1} V_m(x_0,e^{i\omega_1 t}x_1+e^{-i\omega_1 t}x_{-1},\ldots,e^{i\omega_m t}x_m+e^{-i\omega_m t}x_{-m}). \tag{10}$$

Expanding the potential around x_0 we get the following expansion:

$$U_m(x^{(m)})=g_m^0(x_0)+\sum_{\substack{n=-m\\ n\neq 0}}^{m}\frac{g_m^{n,-n}(x_0)}{2!(N+1)}x_n x_{-n}+\sum_{\substack{n_1,\ldots,n_4=-m\\ n_i\neq 0}}^{m}\frac{g_m^{n_1\ldots n_4}(x_0)}{4!(N+1)^2}\times x_{n_1}x_{n_2}x_{n_3}x_{n_4}\delta_{n_1+\cdots+n_4,0}+\cdots. \tag{11}$$

Note that in Eq. (11) there is still conservation of the momentum due to our choice of the potential (10).

To get only the contributions of order $1/\beta$ it is enough to expand the action $S_m(x^{(m)})$ around $x^{(m-1)}$ to the second order [8], so that the result is obtained after a Gaussian integration. The RG equation is

$$S_{m-1}(x^{(m-1)})=S_m(x^{(m-1)})+\tfrac{1}{2}\ln[\det(\mathcal{A})]-J^t\mathcal{A}^{-1}J, \tag{12}$$

with the matrix $\mathcal{A}$ given by

$$\mathcal{A}=\begin{pmatrix} 1+\dfrac{U_m^{(m,-m)}+\mathrm{Re}(U_m^{(m,m)})}{M\omega_m^2} & -\dfrac{\mathrm{Im}(U_m^{(m,m)})}{M\omega_m^2} \\ -\dfrac{\mathrm{Im}(U_m^{(m,m)})}{M\omega_m^2} & 1+\dfrac{U_m^{(m,-m)}-\mathrm{Re}(U_m^{(m,m)})}{M\omega_m^2} \end{pmatrix}$$

and

$$J=\begin{pmatrix} \mathrm{Re}(U_m^{(m)}) \\ -\mathrm{Im}(U_m^{(m)}) \end{pmatrix}$$

with the notation,

$$U_m^{(n_1\cdots n_p)}\equiv(N+1)^{p/2}\frac{\partial^p U_m}{\partial x_{n_1}\cdots\partial x_{n_p}}\bigg|_{(x_{n_1},\ldots,x_{n_p})=0}. \quad (13)$$

From Eq. (12) we deduce the flow equation for the potential part of the action:

$$U_{m-1}=U_m+\frac{1}{2\beta}\ln\left[\left(1+\frac{U_m^{(m,-m)}}{M\omega_m^2}\right)^2-\left|\frac{U_m^{(m,m)}}{M\omega_m^2}\right|^2\right] -\frac{(M\omega_m^2+U_m^{(m,-m)})|U_m^{(m)}|^2-\mathrm{Re}(U_m^{(-m,-m)}U_m^{(m)2})}{(M\omega_m^2+U_m^{(m,-m)})^2-|U_m^{(m,m)}|^2}. \quad (14)$$

For the constant background path $x^{(m)}=x_0$ Eq. (14) reduces to the so called local potential approximation (LPA) of the RG flow,

$$U_{m-1}(x_0)=U_m(x_0)+\frac{1}{\beta}\ln\left(1+\frac{U_m^{(m,-m)}(x_0)}{M\omega_m^2}\right). \quad (15)$$

As in Ref. [7], we will use this LPA to compute the ground state energy and first excited energy level of various quantum mechanical system. In this approximation, $U_m(x_0)=V_m(x_0)$ and $U_m^{(m,-m)}(x_0)=V''_m(x_0)$.

To solve the flow of Eq. (15) we have to expand the potential $V_m(x)$ in series and compute the flow of the coupling constants. As a first application we consider the sextic oscillator.

A. Sextic oscillator

We want to compute the ground state energy of the anharmonic oscillator whose potential is

$$V_{N/2}(x)=\frac{M\Omega^2}{2}x^2+\frac{\lambda}{6!}x^6. \quad (16)$$

Note that in quantum mechanics each coupling in a polynomial interaction is a relevant coupling constant. For an even potential the minimum of the effective classical potential is always located at $x_0=0$ in the absence of phase transition in one-dimensional systems. For this reason we expand V_m around $x_0=0$ and define the nth coupling constant at the scale m as

$$g_m^{(n)}=\frac{d^nV_m(x_0)}{dx_0^n}\bigg|_{x_0=0}. \quad (17)$$

The equation for the first coupling constant is

$$g_{m-1}^0=g_m^0+\frac{1}{\beta}\ln\left(1+\frac{g_m^{(2)}}{M\omega_m^2}\right). \quad (18)$$

The value of the ground state energy is given by $E_0=g_0^0=V_0(0)$, which is the minimum of the effective classical potential. The flow of the quadratic coupling constants is

$$g_{m-1}^{(2)}=g_m^{(2)}+\frac{1}{\beta}\frac{g_m^{(4)}}{M\omega_m^2+g_m^{(2)}}. \quad (19)$$

The particular value $g_0^{(2)}$ corresponds to the mass gap or the inverse correlation length in statistical mechanics language. Then it is well known that the first exited energy level can be deduced from the relation $E_1-E_0=\sqrt{g_0^{(2)}}$.

The general formula for the other coupling constants is given in Eq. [7] and recalled below:

$$g_{m-1}^{(k)}=g_m^{(k)}+\frac{1}{\beta}\left[\sum_p(-1)^{p-1}P_m(0)^p \times\left(\sum_{\alpha_1+\cdots\alpha_p=k,\alpha_i\overline{m}0}\frac{k!A_p}{p}\frac{g_m^{(\alpha_1+2)}}{\alpha_1!}\times\cdots\frac{g_m^{(\alpha_p+2)}}{\alpha_p!}\right)\right],$$

where A_p is the combinatorial factor of $g_m^{(\alpha_1+2)}/\alpha_1!\times\cdots g_m^{(\alpha_p+2)}/\alpha_p!$ in the series expansion of $[V''_m(x_0)]^p$ in power of x_0 and $P_m(0)=1/(M\omega_m^2+g_m^{(2)})$.

Tables I and II display the values of the ground state energy and the first excited energy level for various values of the coupling constant λ.

TABLE I. Ground state energy and first excited energy level of the sextic oscillator for $M\Omega^2=1$.

λ	$E_{0,\mathrm{exact}}$	$E_{0,\mathrm{RG}}$	$E_{1,\mathrm{exact}}$	$E_{1,\mathrm{RG}}$
7.2	0.5154	0.5152	1.5954	1.5956
72	0.5869	0.5847	1.9504	1.9428
720	0.8048	0.7958	2.8749	2.8439
7200	1.2819	1.2610	4.7566	4.6848

TABLE II. Ground state energy and first excited energy level of the sextic oscillator for $M\Omega^2=-1$.

λ	$E_{0,\mathrm{exact}}$	$E_{0,\mathrm{RG}}$	$E_{1,\mathrm{exact}}$	$E_{1,\mathrm{RG}}$
72	0.5434	0.1095	1.3006	0.880
720	0.6808	0.5302	2.4070	2.2627
7200	1.1791	1.1133	4.4602	4.3991

The numerical solution of the RG flow shows a good convergence for $N=10^8$ and $\beta=10^5$. The truncation of the potential at the order six gives the best approximation. Adding more coupling constant does not improve the result on the contrary (see also Ref. [7]).

B. Periodic cosine potential

In this section we extend the application of the RG formalism to a quantum system in a nonpolynomial potential. We choose a cosine potential [11] whose action is defined as

$$S(x)=\int_0^{\hbar\beta}dt\left\{\frac{1}{2}M\left[\frac{d}{dt}x(t)\right]^2+\lambda(\cos\alpha x(t)-1)\right\}.$$

This action has the discrete symmetry $S(x+2\pi/\alpha)=S(x)$. We note $\lambda=2\pi/\alpha$ the period length. It is well known that the energy spectrum of a quantum particle is made up of periodic bands. Following Ref. [11] we note $E_n(\varphi)$ the energy of the nth band, with the property $E_n(\varphi+2\pi)=E_n(\varphi)$. In a finite volume $\varphi=\varphi_p=2\pi p/\beta$.

Let H be the Hamiltonian and Z be the partition function of the system. The stationary states are defined by

$$H|\Psi_{n,p}\rangle=E_{n,p}|\Psi_{n,p}\rangle,$$

which leads to the following expression for the partition function:

$$Z=\int_{-\infty}^{+\infty}dx\langle x|e^{-\beta H}|x\rangle=\lim_{L\to\infty}\int_{-L}^{+L}dx\sum_{n,p}|\psi_{n,p}(x)|^2e^{-\beta E_{n,p}}$$

with $L=N\lambda$. Using the following normalization,

$$\int_{-L}^{L}|\psi_{n,p}(x)|^2\,dx=1,$$

as well as,

$$\sum_{n,p}e^{-\beta E_{n,p}}\underset{N\to\infty}{=}N\sum_n\int_0^{2\pi}\frac{d\varphi}{2\pi}e^{-\beta E_n(\varphi)}$$

we obtain the expression

$$Z=N\sum_n\int_0^{2\pi}\frac{d\varphi}{2\pi}e^{-\beta E_n(\varphi)}.$$

And in the zero temperature limit,

$$Z\underset{\beta\to\infty}{=}N\int_0^{2\pi}\frac{d\varphi}{2\pi}e^{-\beta E_0(\varphi)}\simeq Ne^{-\beta E_0(\overline{\varphi})},\tag{20}$$

where $\overline{\varphi}$ is the location of the minimum of the first band.

The partition can be written in terms of the effective classical potential as

$$Z=\int_{-\infty}^{+\infty}dx_0\,e^{-\beta V_{\mathrm{eff}}(x_0)}$$

From Eq. (2) and the periodicity of the action it is clear that the effective classical potential must be also a periodic function and in the zero temperature limit we get

$$Z\underset{\beta\to\infty}{=}N\exp[-\beta V_{\mathrm{eff}}(\overline{x_0})].\tag{21}$$

Equating Eqs. (20) and (21) leads to

$$E_0(\overline{\varphi})=V_{\mathrm{eff}}(\overline{x_0}).$$

To compute the effective classical potential at its minimum we apply the RG equation,

$$V_{m-1}(x_0)=V_m(x_0)+\frac{1}{\beta}\ln\left(1+\frac{V_m''(x_0)}{M\omega_m^2}\right).$$

It is easy to check that the following form for V is preserved by the RG flow:

$$V_m(x)=\sum_{n=0}^{\infty}b_m^n(\cos\alpha x-1)^n.$$

Then for the second derivative we have

$$\begin{aligned}V_m''(x)&=-\alpha^2\sum_{n=0}^{\infty}[(2n^2+3n+1)b_m^{n+1}+n^2b_m^n]\\&\quad\times(\cos\alpha x-1)^n\\&=\alpha^2\sum_{n=0}^{\infty}c_m^n(\cos\alpha x-1)^n.\end{aligned}$$

Starting with the initial potential

$$V_N(x)=A(\cos\alpha x-1)$$

the RG equation is

$$\begin{aligned}V_{m-1}(x)&=V_m(x)+\frac{1}{2\beta}\ln\left(1+\frac{\alpha^2c_m^0}{\omega_m^2}\right)^2\\&\quad+\underbrace{\frac{1}{2\beta}\ln\left(1+\frac{\sum_{n=1}^{\infty}\alpha^2c_m^n(\cos\alpha x-1)^n}{\omega_m^2+\alpha^2c_m^0}\right)^2}_{=I}.\end{aligned}\tag{22}$$

Expanding the logarithmic term yields

TABLE III. Coupling constants of the periodic cosine potential for $\alpha=0.1$.

λ	b_0^0	b_0^1	b_0^2	b_0^3	b_0^4
−1	0.0992	−0.975	−0.0065	0.0035	−0.0021
−10	0.3154	−9.921	−0.0021	0.012	−0.0064

$$I=\frac{1}{\beta}\sum_{n\geqslant 1}\sum_{p\geqslant 1}\frac{(-1)^{p+1}}{p}\alpha^{2p}$$

$$\times\sum_{k_1+\cdots k_p=n}\frac{c_m^{k_1}\cdots c_m^{k_p}}{(\omega_m^2+\alpha^2 c_m^0)^p}(\cos\alpha x-1)^n.$$

Identifying the different orders in the two members of Eq. (22) we get the flow of the couplings b_m^n. The first terms are

$$b_{m-1}^0=b_m^0+\frac{1}{\beta}\ln\left(1+\frac{\alpha^2 c_m^0}{\omega_m^2}\right)\quad\text{with}\ \ c_m^0=-b_m^1,$$

$$b_{m-1}^1=b_m^1+\frac{1}{\beta}\left(\frac{\alpha^2 c_m^1}{\omega_m^2+\alpha^2 c_m^0}\right)\quad\text{with}\ \ c_m^1=-b_m^1-6b_m^2,$$

$$b_{m-1}^2=b_m^2+\frac{1}{\beta}\left(\frac{\alpha^2 c_m^2}{\omega_m^2+\alpha^2 c_m^0}-\frac{\alpha^4 (c_m^1)^2}{2(\omega_m^2+\alpha^2 c_m^0)^2}\right)$$

$$\text{with}\ \ c_m^2=-4b_m^2-15b_m^3.$$

The ground state energy is given by

$$E_0(\overline{\varphi}=0)=b_0^0.$$

Truncating the expansion at the second order we can compute numerically the flow of the couplings to get an approximation of the ground state energy. Some results are given in Tables III and IV for various values of λ and α.

These results show that the effective classical potential is periodic but not flat as asserted in Ref. [12]. Although it is well known that the effective potential is a convex quantity that must be flat if periodic, take care that this property is true for the effective potential defined as a Legendre transform of the generating functional $W[j]$ of connected Green's functions. Actually the classical effective potential [3,4] has not to be convex.

To confirm our statement consider the density of particle [4,10] computed in Ref. [9],

$$\rho(x_a)=Z^{-1}\int dx\langle x|e^{-\beta H}|x\rangle\,\delta(x-x_a)\tag{23}$$

whose very good approximation is

$$\rho(x_a)\approx Z^{-1}\int\frac{dx_0}{\sqrt{2\pi\beta/M}}\frac{\exp[-(x_a-x_0)^2/2a^2(x_0)]}{\sqrt{2\pi a^2(x_0)}}$$

$$\times e^{-\beta V_0(x_0)}\tag{24}$$

with

$$a^2(x_0)=\frac{2}{\beta}\sum_{m=1}^{N/2}\frac{1}{M\omega_m^2+V_m^{(2)}(x_0)}.\tag{25}$$

It is clear that the density of particle has to be periodic $\rho(x_a)=\rho(x_a+\lambda)$ and nonconstant, so that by inspection of Eq. (24) $V_0(x_0)$ has to be nonconstant and periodic.

TABLE IV. Coupling constants of the periodic cosine potential for $\alpha=1$.

λ	b_0^0	b_0^1	b_0^2	b_0^3	b_0^4
−1	3.098	−9.187	−0.24	0.15	−0.09
−10	0.930	−0.653	−0.42	2.08	−8.21

TABLE V. Ground state energy of the coupled oscillator in the symmetric case $a_{11}=a_{22}=1$. In every entry, the upper number is the exact energies obtained from [13], whereas the lower number is our RG result.

$\lambda\backslash a_{12}$	1	0.2	−0.2
0.05	1.0843	1.0692	1.0613
	1.0837	1.0648	1.0647
0.1	1.1502	1.1250	1.1114
	1.1485	1.1182	1.1078
1	1.7242	1.6332	1.5802
	1.7044	1.6127	1.5615
10	3.301	3.0753	2.9396
	3.230	3.0160	2.8840

C. Pair of coupled oscillator with quartic coupling

In this section we extend the one quantum particle RG formalism to a system of two particles in interaction and compare with some exact results [13].

Consider the following two particles model with action written in continuous time:

$$S=\int_0^\beta dt\left\{\frac{M_1\dot{x}_1^2}{2}+\frac{M_2\dot{x}_2^2}{2}+V(x_1,x_2)\right\}.$$

We define $V_m(x_0^1,x_0^2)$ the running potential at scale m for a two particle system. Let $V_m^{i,j}$ the second derivative of V_m with respect to x_0^i and x_0^j. Similar to the one particle case the RG equation is straightforwardly derived,

$$V_{m-1}(x_0^1,x_0^2)=V_m(x_0^1,x_0^2)+\frac{1}{\beta}\ln\left[\left(1+\frac{V_m^{11}(x_0^1,x_0^2)}{M_1\omega_m^2}\right)\right.$$

$$\left.\times\left(1+\frac{V_m^{22}(x_0^1,x_0^2)}{M_2\omega_m^2}\right)-\left(\frac{V_m^{12}(x_0^1,x_0^2)}{\sqrt{M_1M_2}\,\omega_m^2}\right)^2\right].$$

Choosing a quartic potential

$$V(x_1,x_2)=\lambda(a_{11}x_1^4+2a_{12}x_1^2x_2^2+a_{22}x_2^4),$$

TABLE VI. First excited energy level of the coupled oscillator in the symmetric case $a_{11}=a_{22}=1$.

$\lambda \backslash a_{12}$	1	0.2	-0.2
0.05	2.2388	2.1972	2.1746
	2.2372	2.1852	2.1850
0.1	2.414	2.3471	2.3094
	2.408	2.3361	2.3152
1	3.8304	3.6073	3.4704
	3.7511	3.4871	3.3421
10	7.527	6.9887	6.6476
	7.233	6.771	6.4612

it is easy to derive the flows of the different coupling constants around the point $x_0^1=0$, and $x_0^2=0$ in order to compute the ground state energy. We omit to write the long expressions of the RG flows for the coupling constants and only report in Tables V, VI, and VII the results for the ground state energy and first excited energy level as well as the exact results for comparison [13].

The computations have been performed by truncating the series expansion of the potential at the sixth order. Again our results are very accurate for small couplings and accurate to a few percent for large couplings.

III. RENORMALIZATION GROUP AT FINITE TEMPERATURE

A. Perturbative renormalization group series

At finite temperature the derivation of the RG equation needs some precautions. First of all as shown in Ref. [8], and recalled in the first section this equation can only be derived consistently for a constant background path x_0. Second as shown in Ref. [7], we can no more neglect corrections of order higher than $1/\beta$. In Ref. [7], we showed that the correct formula at finite temperature for the flow of the running potential is given by

$$\begin{aligned} V_{m-1}(x_0) &= V_m(x_0)+\frac{1}{\beta}\ln\left(1+\frac{V_m^{(2)}(x_0)}{\omega_m^2 M}\right) \\ &\quad +\frac{1}{\beta}\ln\Bigg\{1+\sum_{n\geqslant 2}\frac{n!}{\beta^{-1}}\sum_{k_1p_1+\cdots+k_np_n=n}(-)^{k_1+\cdots+k_n} \\ &\quad \times\frac{[V_m^{(2p_1)}(x_0)]^{k_1}}{k_1!(p_1!)^{2k_1}}\cdots\frac{[V_m^{(2p_n)}(x_0)]^{k_n}}{k_n!(p_n!)^{2k_n}}P_m^n\Bigg\}, \end{aligned} \tag{26}$$

where $P_m=1/[\omega_m^2 M+V_m^{(2)}(x_0)]$.

This equation has not the closed form of the zero temperature RG equation (15) as it contains an infinite number of terms.

Let us quickly review the border cases.

TABLE VII. Ground state energy of the coupled oscillator in the dissymmetric case $a_{11}=0.4$, $a_{22}=1$.

$\lambda \backslash a_{12}$	1	0.2	-0.2
0.05	1.0669	1.0509	1.0424
	1.0667	1.0512	1.0428
0.1	1.1206	1.0933	1.0782
	1.1250	1.0871	1.0721
1	1.6123	1.5043	1.4379
	1.5961	1.4854	1.4274
10	3.0175	2.8165	2.5580
	2.8826	2.6552	2.3451

1. Infinite temperature

For a large temperature, the quantum fluctuations are small and the system is close to the classical one. The flow of the potential stays near the classical one (the potential energy of the action) and will be obtained after a relatively small number of iterations of the RG equation. In particular in the limit $\beta\to 0$, $V_m^{(2)}(x_0)/\omega_m^2 M$ and P are of order β^2 and we obtain

$$V_{m-1}(x_0)=V_m(x_0),$$

a running potential constant along the flow. As a consequence the quantum partition function reduces to the classical one.

2. Zero temperature

In this opposite case due to quantum fluctuations the effective classical potential is expected to be different from the classical one and will be obtained after a huge number of iterations of the RG equation (typically 10^8 for $\beta=10^5$). The higher loop contributions are negligible, then we can extract informations for large coupling constants. In particular, in the limit $\beta\to\infty$ the propagator P_m is of order $1/V_m^{(2)}(x_0)$. Then, keeping only the one loop contribution in Eq. (26) we recover the closed form (15):

$$V_{m-1}(x_0)=V_m(x_0)+\frac{1}{\beta}\ln\left(1+\frac{V_m^{(2)}(x_0)}{\omega_m^2 M}\right).$$

3. Finite temperature

For finite β the partition function

$$Z=\int\frac{dx_0}{\sqrt{2\pi\hbar\epsilon/M}}\exp[-\beta V_0(x_0)]$$

is no more dominated by the minimum of the effective classical potential.

Thus, at finite temperature, the computation of the partition function requires the whole knowledge of the effective classical potential, and not only its value at the minimum. We will not compute the ground state, but rather the free energy $\ln Z/\beta$ of the system.

TABLE VIII. Free energy of the anharmonic oscillator for $M\Omega^2=1$. F_{RG} is the perturbative RG computation and F_{var} is the Feynman-Kleinert variational computation [3,4].

λ	β	F_{RG}	F_{var}	F_{exact}
2.4	1	0.228 69	0.226 08	0.226 07
2.4	5	0.546 33	0.559 15	0.558 67
12	1	0.486 30	0.492 68	0.492 58
12	10	0.671 75	0.700 93	0.696 29
12 000	0.1	2.679 04	2.699 7	2.68 34
12 000	10	5.252 88	5.452 5	5.319 9

To do so, we first write a perturbative expansion of the RG equation (26) truncated to the fourth order in $1/\beta$:

$$V_{m-1}(x_0)=V_m(x_0)+\frac{1}{\beta}\ln\left(1+\frac{V_m^{(2)}(x_0)}{\omega_m^2 M}\right)-\frac{1}{2\beta^2}\frac{V_m^4(x_0)}{P_m^2}$$

$$-\frac{1}{\beta^3}\left(\frac{1}{6}\frac{V_m^6(x_0)}{P_m^3}+\frac{1}{8}\frac{[V_m^4(x_0)]^2}{P_m^4}\right)$$

$$-\frac{1}{\beta^4}\left(\frac{1}{24}\frac{[V_m^4(x_0)]^3}{P_m^6}+\frac{1}{12}\frac{V_m^4(x_0)V_m^6(x_0)}{P_m^6}\right).$$

By deriving this equation we also get an infinite set of RG equations for the successive derivatives $V_m^{(k)}(x_0)$ of the running potential. For the numerical computations, we will neglect all the derivatives of order more than six.

Then, we compute numerically, the flow of the successive derivatives up to the sixth order of the potential in different point x_0. It allows to reconstruct an approximation of the whole effective classical potential up to the fourth order in $1/\beta$, and then to compute the free energy of the system.

The results for a quartic initial potential are reported in Table VIII, for various values of the coupling constant λ.

The free energy computed with the RG method is denoted F_{RG}. For comparison, we report also F_{exact} and F_{var} the free energy computed with the Feynman-Kleinert variational method [3,4].

The results obtained with the RG method are not far from the exact free energy, but are clearly less good than the variational method. The trouble comes from the truncation of the running potential at the sixth order, as well as the truncation at the fourth order in $1/\beta$. An attempt to improve these results by increasing the order of the expansion, would be too cumbersome. It is quite surprising that the RG method is very powerful in the most complex case (zero temperature) where quantum fluctuations are very important whereas the results are less accurate at finite temperature where quantum fluctuations are less relevant. In this last case we should expect the truncation of the expansion of the potential to be a good approximation. The trouble here is that, at finite temperature, we have to rebuild the whole effective classical potential to compute the free energy. In this case, our truncation is too rough to give an accurate approximation of the true effective classical potential. In the zero temperature case, we just need to fit the effective classical potential at its minimum, which for quadratic [7] or sextic interaction appears to be well approximated by a sextic polynomial in x_0.

As it is difficult to avoid the truncation of the set of RG equations for the derivatives of the running potential, we can at least, avoid the truncation in power of $1/\beta$. In the following, we propose another method that tries to improve the variational Feynman-Kleinert method.

B. Variational renormalization group equation

In the Feynman-Kleinert (FK) method, one tries to find a quadratic potential at each point x_0 fitting at best the effective classical potential. One can improve this procedure by looking for a quadratic potential $\Omega_m^2(x_0)x^2$ fitting $V_m(x_0)$ at each step of the renormalization group flow. Then by improving in such a manner the FK method, one will take into account some contributions of the Kleinert's variational perturbation expansion [4].

The derivation of the variational RG equation was done in Ref. [7]:

$$V_{m-1}(x_0)=\frac{1}{\beta}\ln\left(1+\frac{\Omega_m^2(x_0)}{\omega_m^2}\right)-\frac{1}{\beta}\frac{\Omega_m^2(x_0)}{\Omega_m^2(x_0)+\omega_m^2}+V_{\alpha_m^2}(x_0), \tag{27}$$

where $\Omega_m^2(x_0)$ is the variational parameter satisfying the integral equation:

$$\Omega_m^2(x_0)=\int\frac{dx}{\sqrt{2\pi a_m^2}}\,\frac{x}{2}\exp(-x^2/2)V_m'(x_0+\sqrt{a_m^2(x_0)}x) \tag{28}$$

with

$$a_m^2(x_0)=\frac{2}{\beta}\frac{1}{\Omega_m^2(x_0)+\omega_m^2}$$

and

$$V_{a_m^2}(x_0)=\int\frac{dx}{\sqrt{2\pi a_m^2}}\exp[-(x-x_0)^2/2a_m^2(x_0)]V_m(x). \tag{29}$$

To perform an analytic computation, we expand $V_m(x)$ in the right hand side of Eqs. (28) and (29) in a series of $(x-x_0)^kV_m^{(k)}(x_0)$. Keeping only the derivatives up to the order V_m^4 allows a complete analytic computation. This means that the running potential is fitted at each point x_0 by a polynomial of order four.

Let $X=a_m^2$, the integrations in Eqs. (28) and (29) yields

$$V_{a_m^2}(x_0)=V_m(x_0)+\tfrac{1}{2}V_m^{(2)}(x_0)X-\tfrac{1}{8}V_m^{(4)}(x_0)X^2,$$

$$\Omega_m^2(x_0)=V_m^{(2)}(x_0)+\tfrac{1}{2}V_m^{(4)}(x_0)X.$$

Equating this last result to $\Omega_m^2=2/\beta a_m^2-\omega_m^2=2/\beta X-\omega_m^2$ leads to a second order equation in X whose solution is

TABLE IX. Free energy of the anharmonic oscillator. $F_{\rm RG}$ is the variational RG computation and $F_{\rm per,var}$ is the perturbative variational result of Kleinert [4,5].

λ	β	$F_{\rm RG}$	$F_{\rm var}$	$F_{\rm per,var}$	$F_{\rm exact}$
0.012	2	0.427 938	0.427 937	0.427 937	0.427 741
2.4	1	0.226 075	0.226 084	0.226 075	0.226 074
2.4	5	0.559 46	0.559 155	0.558 678	0.558 675
12	1	0.492 612	0.492 685	0.492 578	0.492 579
12	5	0.701 25	0.699 431	0.696 180	0.696 118
12 000	0.1	4.500	2.699 7	2.698 34	2.698 34
12 000	10	9.875	5.452 5	5.622 5	5.319 9
480 000	0.1	46.61	18.15	18.047	18.045

$$X=\frac{-[V''_m(x_0)+\omega_m^2]+\sqrt{(V''_m(x_0)+\omega_m^2)^2+4V_m^{(4)}/\beta}}{V_m^{(4)}}. \tag{30}$$

In terms of X, Eq. (27) becomes

$$V_{m-1}(x_0)=V_m(x_0)+\frac{1}{\beta}\ln\left(\frac{\beta X}{2\omega_m^2}\right)-\tfrac{1}{8}V_m^4(x_0)X^2 \tag{31}$$

and the RG flows for the derivatives of the running potential are

$$V'_{m-1}(x_0)=V'_m(x_0)-\frac{1}{\beta}\frac{X'}{X}-\tfrac{1}{4}V_m^4(x_0)X'X,$$

$$V_{m-1}^{(2)}(x_0)=V_m^{(2)}(x_0)-\frac{1}{\beta}\left(\frac{X''}{X}-\frac{X'^2}{X^2}\right)-\tfrac{1}{4}V_m^4(x_0)(X''X+X'^2),$$

$$V_{m-1}^{(3)}(x_0)=V_m^{(3)}(x_0)-\frac{1}{\beta}\left(\frac{X^{(3)}}{X}-\frac{3X''X'}{X^2}+\frac{2X'^3}{X^3}\right)-\tfrac{1}{4}V_m^4(x_0)(X^{(3)}X+3X''X'),$$

$$V_{m-1}^{(4)}(x_0)=V_m^{(4)}(x_0)-\frac{1}{\beta}\left(\frac{X^{(4)}}{X}-\frac{4X^{(3)}X'+3X''^2}{X^2}+\frac{12X''X'^2}{X^3}-\frac{6X'^4}{X^4}\right)-\tfrac{1}{4}V_m^4(x_0)(X^{(4)}X+4X^{(3)}X'+3X''^2),$$

where the derivatives of X are obtained from Eq. (30). Let $P=V''_m(x_0)+\omega_m^2$, and $Y=P^2+4V_m^{(4)}/\beta$,

$$X'=\frac{-V_m^{(3)}+PV_m^{(3)}}{V_m^{(4)}},$$

$$X''=-1+PY^{-1/2}+\frac{4}{\beta}(V_m^{(3)})^2Y^{-3/2},$$

$$X^{(3)}=\frac{12}{\beta}V_m^{(3)}V_m^{(4)}Y^{-3/2}-\frac{12}{\beta}(V_m^{(3)})^3PY^{-5/2},$$

$$X^{(4)}=\frac{12}{\beta}(V_m^{(4)})^2Y^{-3/2}-\frac{72}{\beta}(V_m^{(3)})^2V_m^{(4)}P^2Y^{-5/2}-\frac{12}{\beta}(V_m^{(3)})^4Y^{-5/2}+\frac{60}{\beta}(V_m^{(3)})^4P^2Y^{-7/2}.$$

For the numerical application of these flow equations we consider an initial quartic potential with coupling λ. In Table IX, we report the values $F_{\rm RG}$ of the free energy estimated with the variational renormalization group equation for various values of λ. For comparison we also report the exact value $F_{\rm exact}$, as well as the Feynman-Kleinert variational results [3,4] and the perturbative variational results [4,5].

As seen in Table IX, our method works very well, with better results than the perturbative RG results, for small enough coupling constants. Of course our results cannot compete with a systematic application of the perturbative variational method. For very large coupling constants, the results are very bad, even for large temperature. This is due to the fact that in this case, the higher derivatives coupling constants are not negligible, invalidating our truncation. It would be interesting to extend our method by keeping more derivatives of the running potential. But it needs much more work, since it would imply an equation for X of higher degree than 2 (an equation of degree N, if we truncate at the order $2N$).

Nevertheless, for small coupling constants and small β ($\beta<5$) our results are better than the FK variational method and very close to the exact free energy. Actually, at high temperature, the quantum fluctuations are small and the true effective classical potential is close to the initial bare potential. This means that quantum fluctuations do not influence very much the flow of the coupling constants and our truncations at the quartic order is enough for accurate computations. For smaller temperature, the quantum fluctuations influence more the running coupling constants, which in turn grow too much to justify our truncation.

IV. CONCLUSION

In this paper, we have studied in detail the renormalization group formalism for quantum systems at zero and finite temperature.

At zero temperature, the flow equation for the potential has a closed form that allows to obtain nonperturbatively a very good approximation of the ground state energy of the system, as well as the first excited energy level. It is performed by computing the flow of the coupling constants of the truncated potential, around its minimum. We have applied this method to polynomial interaction, as well as a periodic potential and a two particle system. In the case of the periodic system, we obtain a periodic and nonconvex effective classical potential. Actually, our potential, called in [4] the classical effective potential, is different from the Legendre transform of the generating functional of connected Green's functions.

At finite temperature, the renormalization group equation, is given by a perturbative expansion in $1/\beta$. Moreover, we need, in this case, to compute the whole classical effective potential in order to deduce the free energy of the system, since the partition function is no more approximated by the exponential of the minimum of the classical effective potential. By truncating both the RG equation and the running potential, we obtain numerical results inferior to the ones computed with the Feynman-Kleinert variational method.

As we cannot avoid the truncation of the running potential, we have at least avoided the truncation in $1/\beta$ by setting a variational renormalization group equation leading to an analytic equation for the variational parameters.

Our results are very good for small couplings and small β since in these cases, the flow of the coupling constants does not grow too much due to the small quantum fluctuations. For larger β the growth of the coupling constant needs to take into account much more couplings. This point is under consideration.

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